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Executive Editor
John Melchi
jmelchi@ncsa.uiuc.edu

Managing Editor
J. William Bell
jbell@ncsa.uiuc.edu

Art Director
Carlton Bruett

Illustrators
Carlton Bruett
Luke Wroblewski

Copyeditors
Stephanie Drake
Karen Green

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National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign
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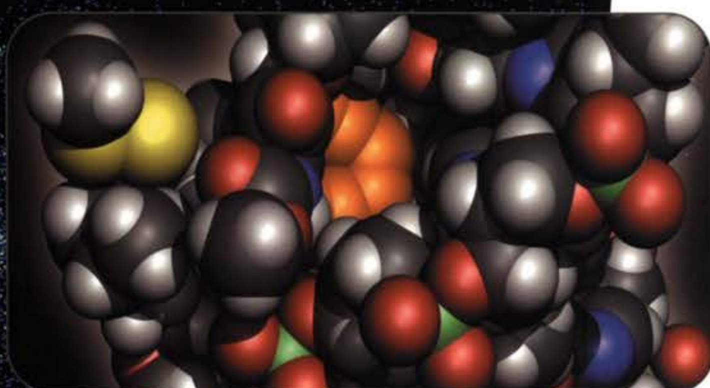
Who we are

The National Computational Science Alliance (Alliance) is a partnership among more than 50 academic, government, and industrial organizations from across the United States to prototype an advanced computational infrastructure for the 21st century. This model infrastructure, called the Grid, will link together advanced supercomputers, visualization environments, and mass storage devices into a powerful, flexible problem-solving environment. This computing environment will be accessed via high-speed networks from anywhere in the country—eventually, the world.

The Alliance is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign with major support from the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. Additional funding for NCSA comes from the state of Illinois, the University of Illinois, industrial partners, and other federal agencies.

Cover

Model of esperamicin A1 with the warhead portion in orange. Using NCSA's SGI Origin2000, a research team at New York's Hamilton College studies enediyne antibiotics such as esperamincin and contributes to knowledge of new cancer treatments.



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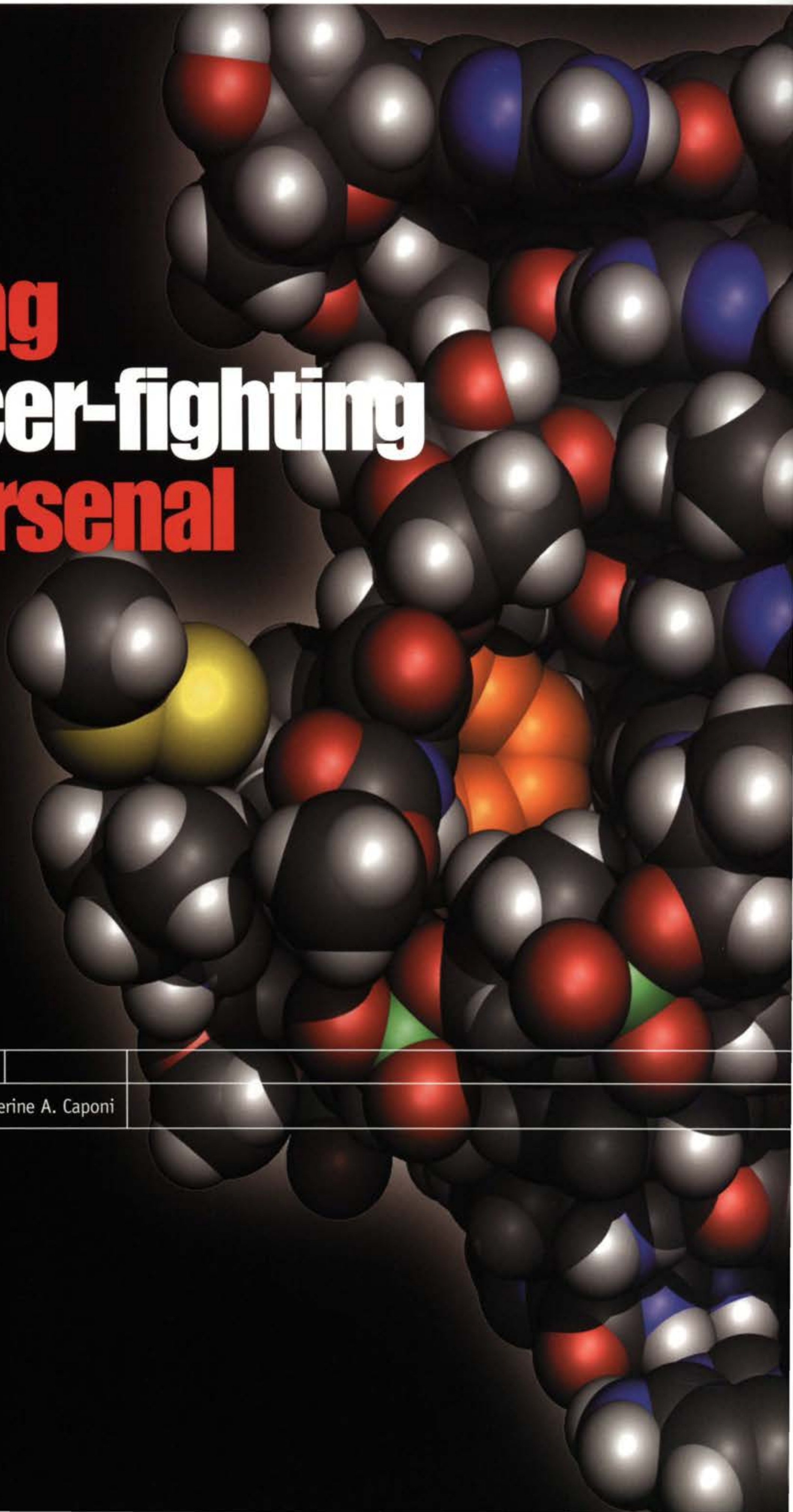
Hamilton College undergrads study natural "biological warheads" on an Alliance SGI Origin2000—and experience the realities of research science first-hand.



by

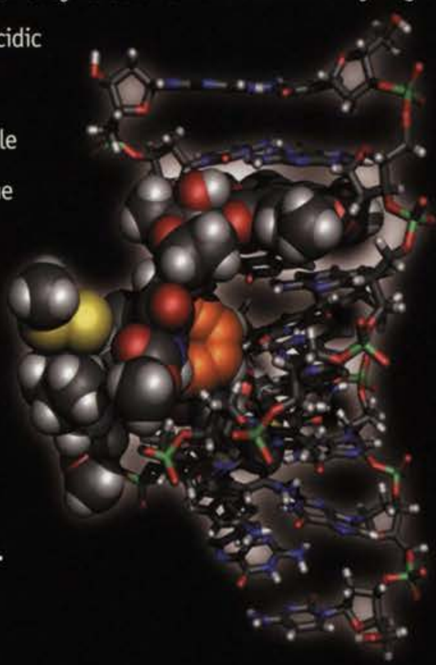
Katherine A. Caponi

Model of esperamicin A1 with the warhead portion displayed in orange.

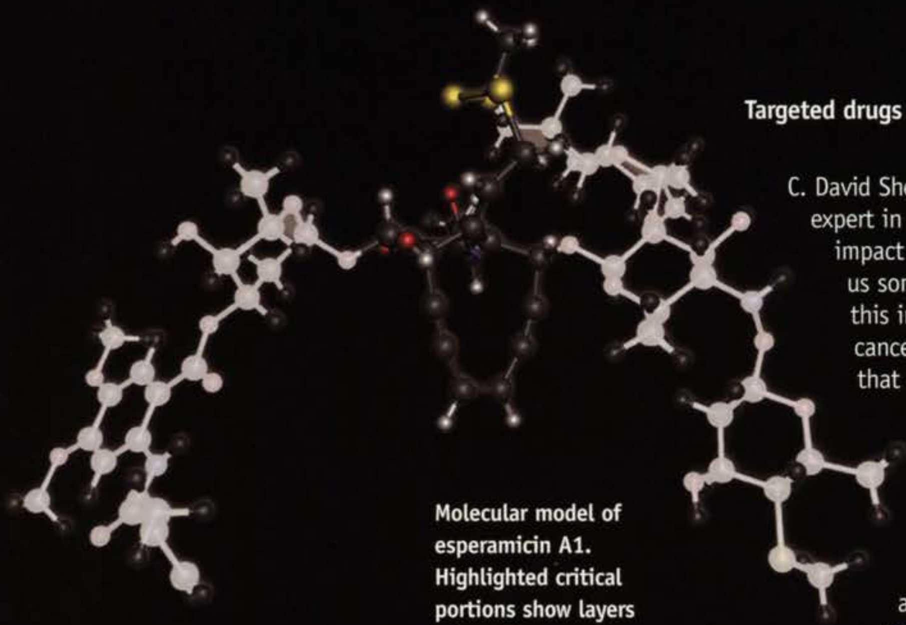
NCSA is arming a team of young scientists with the supercomputing resources necessary to engage in the battle against cancer. This team of undergraduate physical, biological, and computational chemists at New York's Hamilton College joins the front line in computational research on enediynes, naturally occurring molecules commonly called biological warheads for their ability to bind to and split tumors' DNA backbones. Using NCSA's SGI Origin2000 supercomputer, the students are contributing knowledge of new cancer treatments and using computational chemistry in an authentic team research setting.

Scientists became interested in the antitumor activity of enediyne antibiotics such as dynemicin, calicheamicin, and esperamicin because of the molecules' low thermal barriers to Bergman cyclization. Bergman cyclization is a reaction in which the enediyne converts to an intermediary benzene diradical, an aromatic ring missing two carbon-hydrogen bonds. When the molecule is in the intermediary diradical state, it can forcibly extract hydrogen from deoxyribose carbons to split DNA, resulting in the death of cancerous cells.

The temperature barrier is the amount of energy that must be applied to the molecule to cause a reaction. This level is particularly important to drugs' effectiveness because it determines whether Bergman cyclization will occur at human body temperature. Many scientists are trying to synthesize or computationally design molecules that only cyclize when they've taken on an additional hydrogen ion, a process that occurs readily in acidic solutions. The challenge is to find or create an enediyne-containing molecule that is completely unreactive under the normal pH of a healthy cell, yet takes on an additional hydrogen ion in acidic cancerous cells and becomes reactive.



Esperamicin binds to DNA just before Bergman cyclization.



Molecular model of esperamicin A1. Highlighted critical portions show layers where the research team performed the most intensive calculations.

Targeted drugs from targeted computing

C. David Sherrill of the Georgia Institute of Technology, an expert in the field of enediyne chemistry, reacted to the impact of the Hamilton team's work, "[Their research] tells us something about exactly how these drugs react, and this information may be useful in designing new anti-cancer drugs that are more effective. It is very exciting that computational simulations are starting to give us insight into these difficult-to-study molecules."

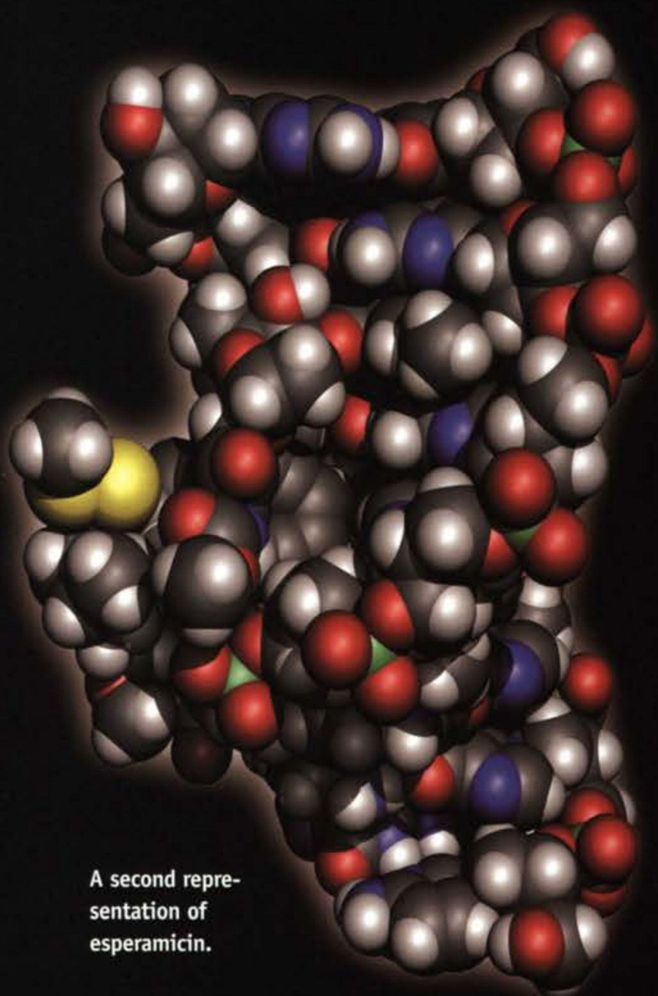
The team at Hamilton is learning to manipulate cyclization temperatures, increasing the chances that a more effectively targeted class of antibiotics with low toxicity to healthy cells will be developed. The ultimate goals of the undergrads are to observe the drug-induced extraction of hydrogen molecules, which splits the DNA; to find and manipulate the thermal barrier for cyclization; and to view the natural processes that occur in conjunction with the reaction.

To accomplish their goals, the team is using complex calculations with pinpoint accuracy on the warhead, or the six-carbon enediyne portion, of the molecule. They perform slightly less complicated calculations on the next crucial layer, the body of the molecule, which is the portion tied up in rings right around the enediyne. The body is critical in lowering the barriers for cyclization. The molecule's body also contains the triggering mechanism that prevents cyclization before the drug is located in DNA. The arms of the molecule, which require the lowest level of calculation, are side chains that jut off the body and help a drug bind to DNA.

Applying varying levels of theory to different parts of the molecule is called the ONIOM method. ONIOM is a computational method developed by Keiji Morokuma, a computational chemistry pioneer at Emory University. ONIOM, created in part using Alliance supercomputing resources, lowers costs of research by applying supercomputing techniques with varying levels of precision to different layers of the molecule studied. This strategy allows the Hamilton team to focus their efforts and resources on the warhead parts of the molecule that are most important to understanding the diradical formation.

Basic training in computational chemistry

Hamilton's Dreyfus postdoctoral teaching fellow Steven Feldgus is principal investigator on the project, which has used about 40,000 hours of supercomputing time and was recently awarded an additional 15,000 hours. He has worked extensively with NCSA resources in the past, beginning with projects in graduate school, and has applied for and used over 100,000 supercomputing hours for multiple projects in the last three years.



A second representation of esperamicin.

Feldgus began work on the enediyne project during the spring 2001. He performed all beginning calculations between January and mid-May and then stepped into an almost purely advisory role, training the undergraduates and supervising their computations.

He said of the project, "Even though some of our students are freshmen and sophomores, we've got them working on a real chemical problem using world-class computers, and we've got them hooked. When it comes to getting students to learn and get excited about research, we're doing as well as anyone. And that's the most satisfying part of this work for me. And who knows? Perhaps one of these students will go on and someday make a major breakthrough in the field. That would just be gravy."

Chantelle Rein, David Kelland, and Beth Hayes joined the project as the undergraduate team in summer 2001. Rein began studying the effects of substituting different parts of esperamicin molecules, one class of enediyne antibiotics, to raise and lower the barriers to Bergman cyclization. Rein presented the results of her work at the Sanibel Symposium, a quantum chemistry conference in St. Augustine, FL, this February. As the lone freshman on the team, Kelland's objective is to test the accuracy of the ONIOM method applied to Bergman cyclization by comparing ONIOM results to enediynes where the thermal barriers to cyclization are already known experimentally. Hayes is looking at possible reaction pathways between oxygen and a small diradical molecule.

George Shields, a co-principal investigator for the project, says that this hands-on approach to education is an essential element in turning students into scientists, "We feel that the best kind of teaching stems from the mentoring and one-on-one interactions between faculty and students in a small research group. Science has always worked best with the apprenticeship model, and we give undergraduates a chance to find out if they want to become research scientists before they have to make a decision on whether to attend graduate school."

This research is supported by the National Science Foundation and the Camille and Henry Dreyfus Foundation.

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For further information:

http://www.chem.hamilton.edu/faculty/feldgus.html

Team members

Steve Feldgus
Beth Hayes
David Kelland
Chantelle Rein
George Shields

Models in a flash

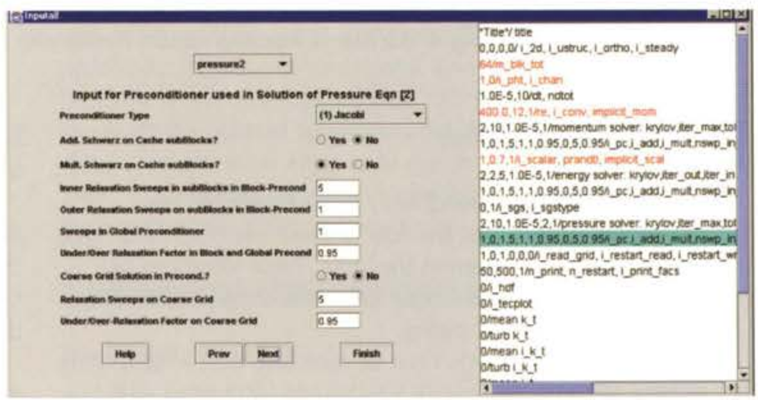
by
J. William Bell

NCSA and Alliance researchers provide Shell Oil Company with code and expertise for modeling refining and production equipment—and in less than a week set up the first Linux cluster in Shell's oil products and chemicals research areas.

Vacuum flashers—they almost sound made up. Something a movie fighter pilot barks about being damaged in a dogfight. Something that allows a DeLorean to travel through time.

Outside the movies, however, vacuum flashers are a critical, elementary part of many applications in the petroleum and chemical industry. These devices are nothing more than vessels in which varying atmospheric pressure allows products to be distilled from another substance. Vacuum distillation prevents decomposition at the point of vaporization, and the separation into components yields useful end products or elements that can be used in other processes.

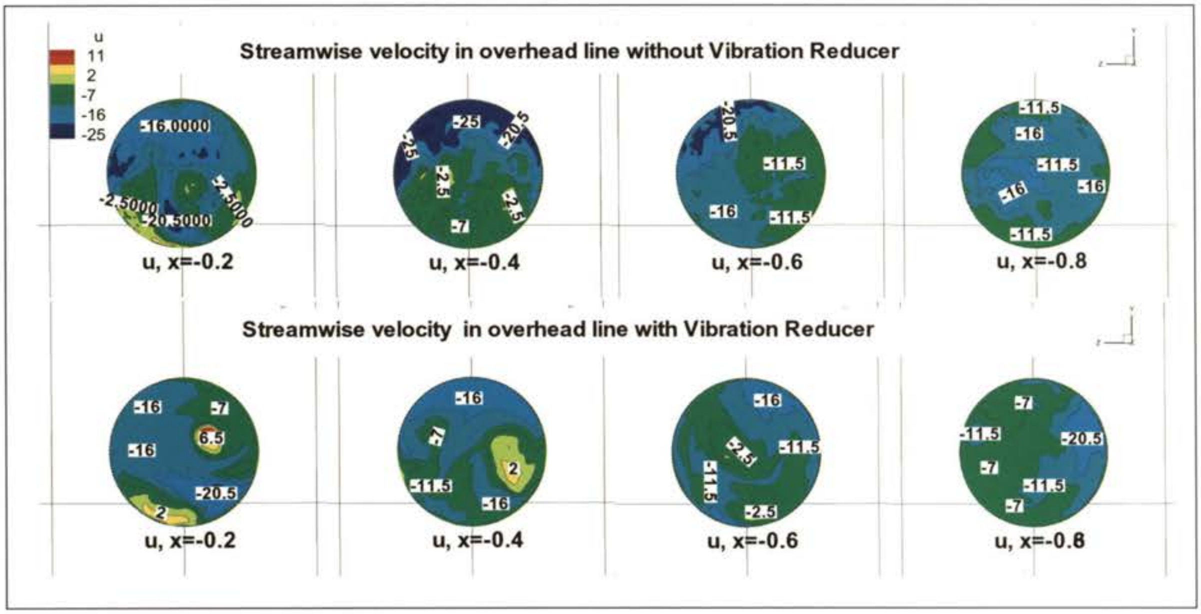
Regardless of the initial substance and the eventual products, vacuum flashers are home to a wicked fluid dynamics environment. Liquids and gases flowing among one another trigger dramatic fluctuations in pressure and velocity—fluctuations we know as turbulence. Understanding this turbulence, its impact, and methods of combating it is not only a great research challenge. It will also impact the industrial bottom line by both reducing the deterioration of vacuum flashers and increasing the flashers' efficiency.



GenIDLEST software interface.

In an effort to come to terms with turbulence, NCSA recently completed an extensive project with Shell Oil Company. Working under the auspices of NCSA's Private Sector Program, a research team modeled a vacuum flasher that Shell uses in chemical manufacturing. The team used an NCSA massively parallel computational fluid dynamics code known as GenIDLEST to capture with remarkable precision both the complex geometry of the vessel and the time-dependent characteristics of the turbulent flows. While they were at it, the team set up a Linux computing cluster dedicated to Shell computational fluid dynamics research. With standardized software that is now part of the Alliance's Cluster-in-a-Box software package and off-the-shelf computers, the cluster was up and running in a matter of days.

"We spend a lot of money maintaining commercial tools for our research and technical service projects," says Raghu Menon, a Shell researcher who has collaborated with NCSA for years and is Shell's principal investigator on the application. "But problems like modeling time-dependent turbulence accurately and solutions like the new Linux cluster require relationships like that with NCSA. This relationship is very exciting. The power is apparent."



Streamwise velocity of the flow in modeled vacuum flasher with and without vibration reducer.

A solution and a mystery

Overhead lines carry vapors away from vacuum flashers. Researchers believe that the flow in these overhead lines cause structural vibrations seen in the units. These vibrations, if unmitigated, can cause fatigue failures in the vacuum flashers' nozzles and associated piping.

Much of this vibration can be overcome with what is aptly called a vibration reducer. "It's just a pipe with holes in it that provides resistance to the flow in the flasher and dampens the resonance between the fluid and the flasher at the right frequency," says Danesh Tafti. Tafti was a research scientist at NCSA for 10 years before taking a faculty position in the mechanical engineering department at Virginia Tech in 2002. He continues research for the Alliance, developing GenIDLEST for the academic and industrial community at large.

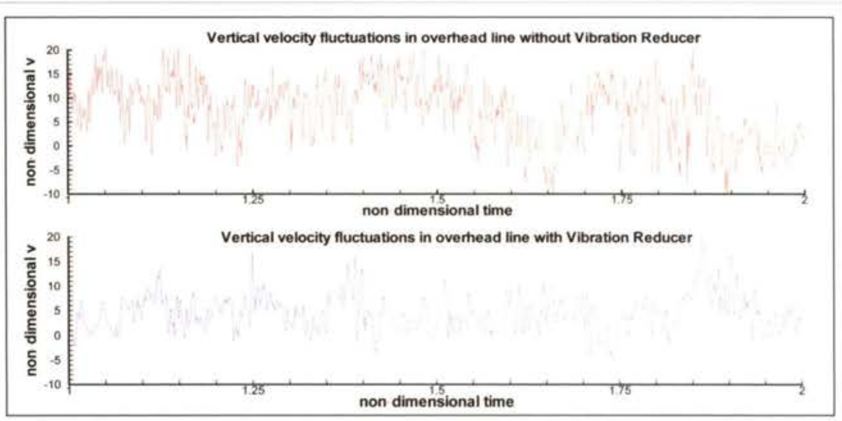
The team from NCSA and Shell used their model to isolate the most energetic modes in the flow. Then the team members could see the vibration reducer in action, suppressing these modes and thus allaying vibrations. They also found that the vibration reducer significantly affects the variation in pressure at points in the flow. The difference in pressure between two such points is known as a pressure drop.

"The same phenomenon responsible for the vibrations also increases the pressure drop through the vacuum flasher. This increased pressure drop is detrimental to the process. It limits the capacity and requires additional energy input, which increases the company's energy costs. The vibration reducer, in addition to suppressing vibrations, decreases the pressure drop and significantly improves the process economics," Menon says.

The vibration reducer also introduces a mystery. Researchers aren't sure how the simple little gadget works. "At this point, we don't know the exact mechanism, we only know the effects," Tafti says. "It's isolating the exact mechanism that we'd like to continue to pursue."

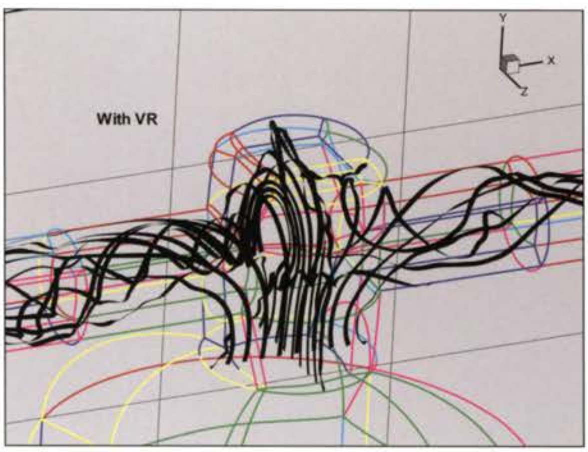
Also RANS

Until their work with NCSA, Shell relied on a common computational fluid dynamics method known as RANS or Reynolds Averaged Navier-Stokes. This approach has its benefits. It's cheap computationally, and it gives researchers an overall understanding of the behavior of the flow rather quickly. It does not, however, capture the wildly random, time-dependent nature of large-eddy, or very turbulent, flows like those found in a vacuum flasher.



Vertical velocity vibrations in modeled vacuum flasher with and without vibration reducer.

Flow in modeled vacuum flasher without vibration reducer.



Flow in modeled vacuum flasher with vibration reducer.

GenIDLEST is designed for just such flows. Instead of time-averaging the flow and treating it as steady, GenIDLEST solves the time-dependent Navier-Stokes equations—which are the Rosetta Stone for fluid dynamics, the base equations that make possible understanding and modeling a system. The code describes the flow at every moment in all its complexity.

To do this work at the high flow velocities encountered in the vacuum flasher, researchers at Shell and NCSA had to use a fine-grained mesh that demanded that the calculations be run at about 1.6 million points throughout the model vacuum flasher's complex shape. This arrangement was demanding—the initial run required about 10,000 hours on NCSA's SGI Origin2000 supercomputer—but it showed the team many of the aspects of the flow with more precision than ever before.

"We agreed that this had to be a time-dependent simulation, and that our standard methods wouldn't meet the requirements. It was well beyond our current capabilities and what we do typically," Menon says.

Made to order in less than a week

The model has already shown researchers many of the flow's characteristics—that it is marked by large velocity and pressure fluctuations with a dominant frequency and that introducing a vibration reducer significantly calms that dominant vibration. Nonetheless, Shell researchers would like to know a lot more. To that end, Jeremy Enos, part of the NCSA team, helped install an eight-processor Linux computing cluster at a Shell research facility in Houston in January 2001. The Shell team plans to expand the cluster and install the Alliance's GenIDLEST software in 2002.

Getting the cluster up and running in less than a week was possible only because of OSCAR, the Open Source Cluster Application Resources. This suite of tools and software has everything needed to install, maintain, and use a modest-sized Linux cluster. OSCAR is now a part of the Alliance's larger Cluster-in-a-Box software package.

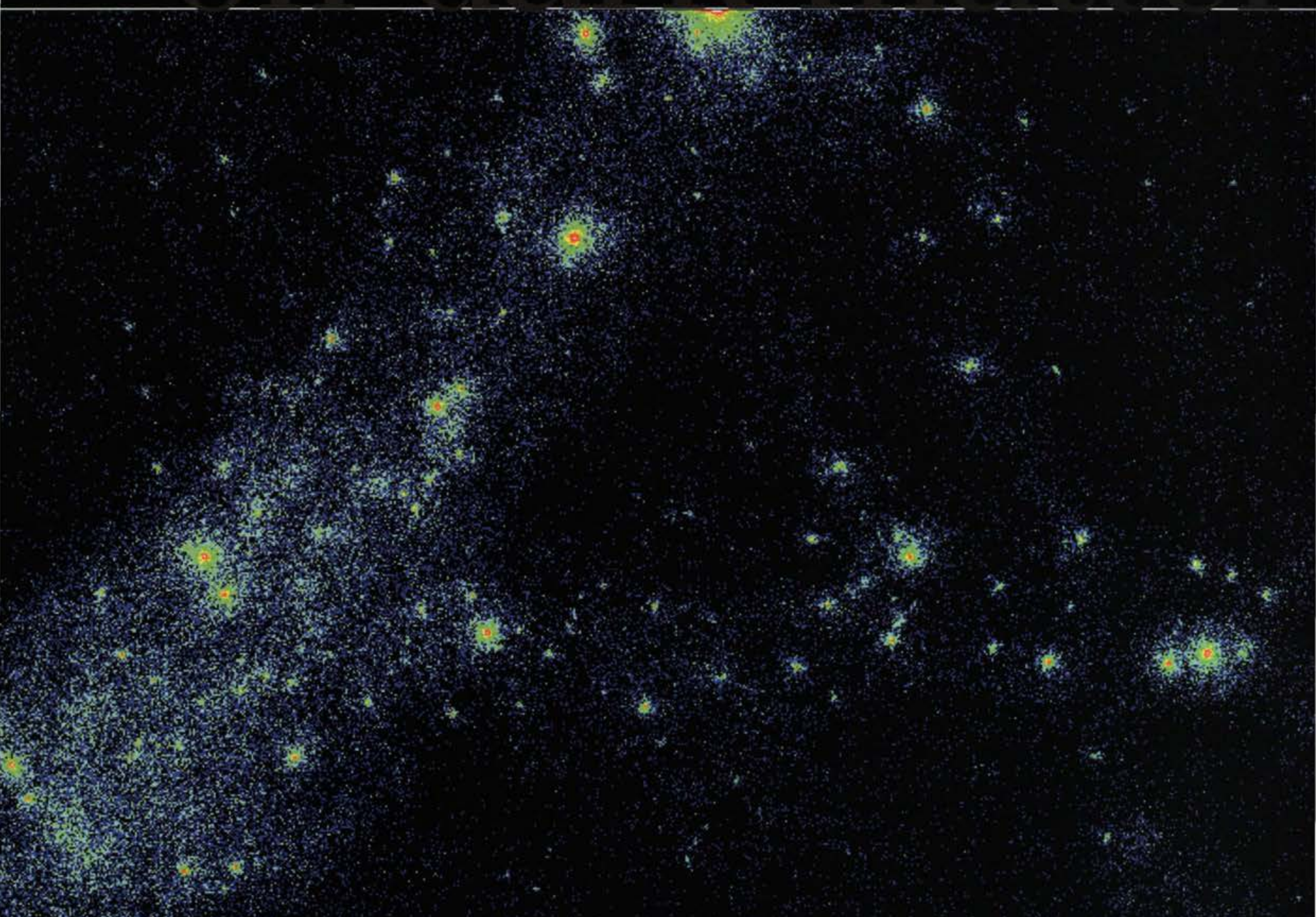
"Danesh and Raghu have been talking about this for years," says Sundaresan Bala, who managed Shell's relationship with NCSA until his recent retirement. "When the time came to update our in-house computational fluid dynamics capability, they saw an opportunity, and they took it. Now we have a cheap, easily installed system and the room to grow. With this system and our other eight or so clusters in other groups at Shell, PC Linux clusters are an important part of our high-performance computing strategy."

Access Online http://access.ncsa.uiuc.edu/CoverStories/genidlest/

For further information:
http://www.ncsa.uiuc.edu/TechFocus/Deployment/CiB/

Team members
Sundaresan Bala
Jeremy Enos
Raghu Menon
Danesh Tafti

Shedding light on dark matter



by

Karen Green

Massive computer simulations give scientists clues to the nature of dark matter.

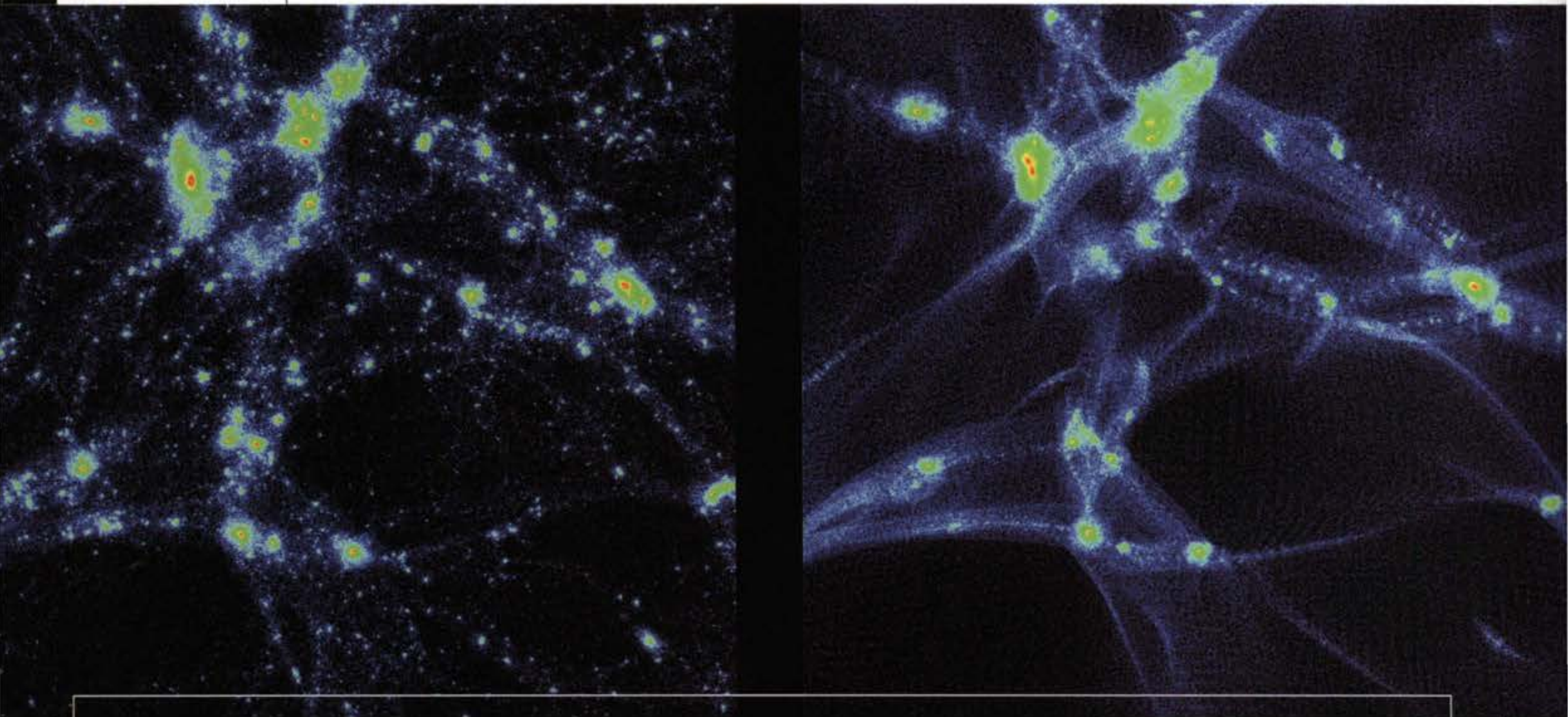
Think of today's astrophysicists as cosmic detectives. As better instruments make it possible to look at clusters of stars and galaxies billions of light years from earth, astrophysicists are able to see back in time to when the universe was relatively youthful. With this vision, they can compare their observations with theoretical simulations that attempt to explain cosmic events in the early universe. These glimpses of the past, as well as the computer simulations, are clues that will hopefully lead to answers to some of the most fundamental questions of science: Why is cosmic material dispersed in clumps rather than distributed evenly across the universe? What is the nature of that mysterious, unseen matter—commonly referred to as dark matter—that makes up most of the universe's mass.

Paul Bode, a research scientist at Princeton University, and Jeremiah Ostriker, a Princeton astronomy professor and a member of the Alliance Cosmology team who also holds the Plumian Professorship of Astronomy and Experimental Philosophy at the University of Cambridge, concern themselves with these questions. They have so far logged 25,000 hours on the Alliance's Platinum Linux cluster at NCSA in an effort to describe the properties of dark matter in ways that fit logically with what other astronomers have observed in the universe.

Scientists have postulated the existence of dark matter for more than 25 years, even though they have never been able to see it. In the observed universe, galaxies and clusters of galaxies spin fast—so fast that they must contain more matter than that which can be seen. The outer portions of spiral galaxies rotate around their galaxy centers with such speed that they would fly apart if only their visible matter were holding them together. Likewise, galaxies inside galaxy clusters move in relation to each other at speeds that are faster than what would be induced by the gravity of the galaxies' visible matter. There simply must be more matter, undetectable to human optics, holding together these spinning disks, scientists theorize.

They coined the term dark matter to describe this invisible mass. Dark matter is believed to surround galaxies in invisible halos. The exact nature of dark matter, including its exact mass, how it interacts with other particles, how fast it moves, and how it obeys the general laws of physics, are questions that still need to be answered. Bode and Ostriker believe that the key is to figure out the characteristics dark matter would need to create a universe that looks like the one we see.

"We may think of these very large cosmological simulations as a means of test driving new fundamental theories of physics," explains Ostriker. "We put into the computer some new, specific but speculative theory, start with initial conditions given by microwave observations of the deep past, and then calculate forward. The test is to see if the final computed universe looks like the real one."



Matter density in an area 10 megaparsecs on each side. The image on the left shows matter density as it would occur if dark matter adhered to the properties of cold dark matter (CDM). At right is the same area with matter density as it would occur in warm dark matter (WDM) theory. WDM produces empty voids, whereas CDM results in many small objects inside these spaces.

"One of the questions we have is: How dense and how energetic would dark matter need to be in order for the universe to be the way it is?" adds Bode. "The density of the universe is not uniform, and we believe dark matter provides the extra gravitational pull to attract more matter together into the dense clumps of galaxies that we observe."

The cold, the warm, and the hot

Current theory describes dark matter in three ways. Cold dark matter (CDM) is highly interactive gravitationally with other matter and has no relativistic speed. That is, it is not moving at a percentage of the speed of light. Computer simulations show that CDM results in a universe much like the one we observe if the simulation is done on a very large, multigalactic scale. However, at smaller scales CDM doesn't fare quite as well, creating simulated galaxies with too many small dense clumps of matter.

"Cold dark matter predicts many dwarf structures (small, rogue galaxies) between the large clumps in a galaxy," says Bode. "That is not what has been observed. "

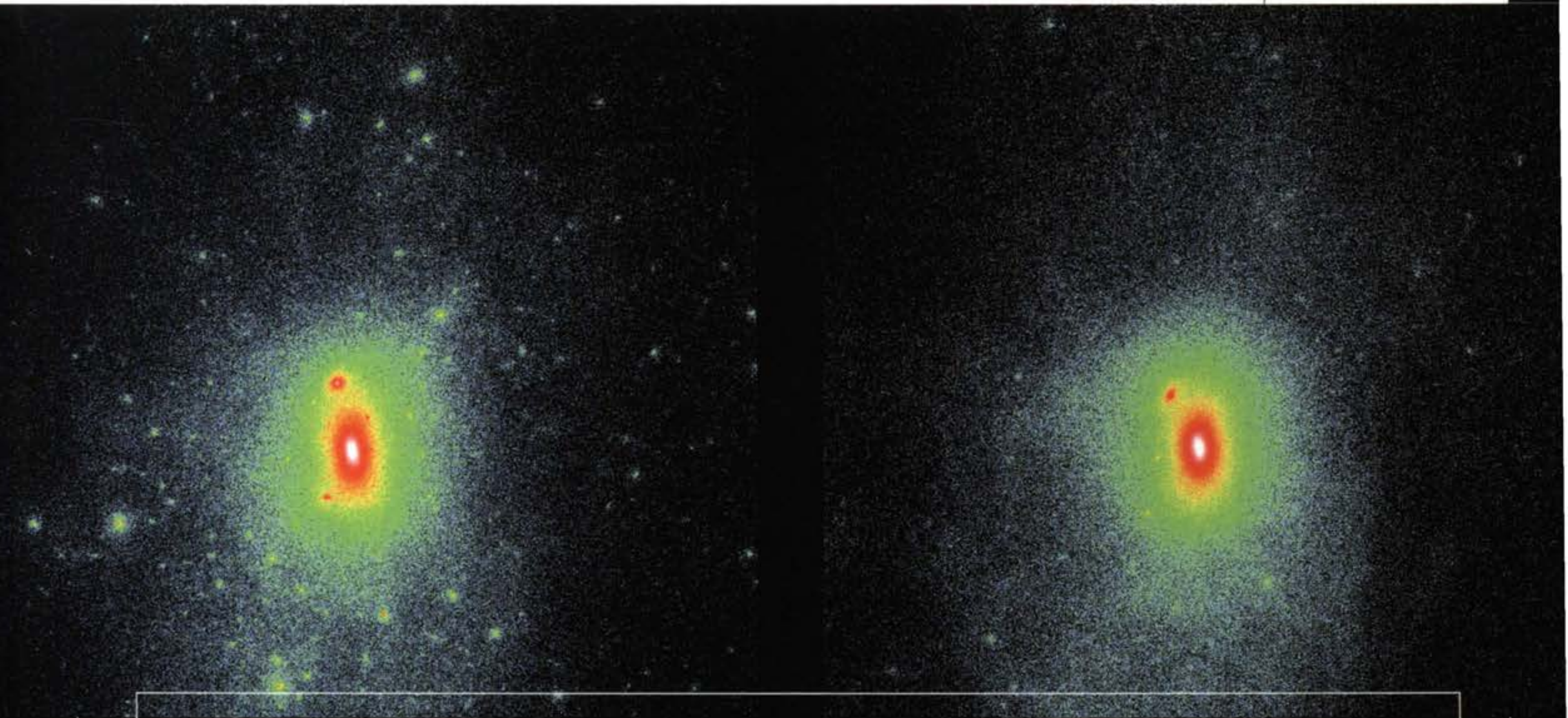
Another possible form of dark matter—hot dark matter—describes a particle like massive neutrinos, which are so weakly interactive that they pass right through regular matter. Scientists have been able to detect neutrinos using huge particle detectors, and neutrinos are believed to be a type of dark matter. However, if most dark matter were neutrinos, matter in the universe would be quite uniformly distributed, explains Bode, and researchers know that it is not.

Ostriker and Bode simulate the formation of galaxy halos using the warm dark matter (WDM) model. WDM is a slight variation of CDM. Because particle velocities are lower, dark matter clumps more with its surroundings than do neutrinos but not as much as CDM particles.

Recreating gravity's effects

The research team's simulations started with a cube of WDM particles initially distributed almost uniformly across a theoretical portion of the universe. For the Linux cluster simulations, this cube consisted of 17 million particles in a grid with 512 cells on each side. The grid area was a randomly picked volume of space, 20 megaparsecs per side. An average galaxy in this grid would occupy about 10 kiloparsecs. The researchers use Tree Particle Mesh (TPM) code to calculate the gravitational force that the particles have on each other over a series of time steps. Over time, particles are attracted to each other and fall toward each other to form dark matters halos. Galaxies form within these dark halos, explains Bode.

The 17 million-particle run took eight days using 128 processors full time. Early in 2002 the team began another set of simulations using 134 million particles in a billion-cell grid. That run is expected to take two months using 128 processors continuously. The TPM algorithm gives Bode and Ostriker a mathematical shortcut for looking at the gravitational force the WDM particles exert on each other. In a world of unlimited computing power, the most straightforward way to compute this force would



Closeup of the dark matter halo surrounding a typical galaxy. In the CDM model (left), the large galaxy has many smaller satellites surrounding it. In the WDM model (right), there are fewer of these satellites. So far, this research suggests that the WDM model fits better with how matter is actually dispersed in the universe. The density of matter increases closer to the center of the halo, from slightly denser than average (blue) to more than a million times denser (white).

be to calculate Newton's law of gravitation on each pair of particles. However, since the current computations involve roughly 10^{16} pairs of particles—that's 10 quadrillion pairs—such calculations are impractical if not impossible. TPM breaks this massive problem down into many smaller ones. It uses a tree code to calculate short-range gravitational forces (forces within the many halos produced by gravity). Then it employs a fixed particle mesh to calculate long-range gravitational forces (forces exerted from outside the halos, including forces in the voids between halos).

"Preliminary indications are that the warm dark matter model could provide a better description of the universe as we've actually observed it compared to the cold dark matter model, in which case it is a clue to what dark matter is," says Bode. "What exactly it is, we still don't know."

The dark matter mystery is still unsolved, but, thanks to more detailed simulations, the clues are coming quickly. With a little more detective work, some answers should be revealed.

This research is supported by the National Science Foundation and the National Computational Science Alliance.

Access Online http://access.ncsa.uiuc.edu/CoverStories/wdm/

For further information:

http://astro.princeton.edu/~bode/

Team members

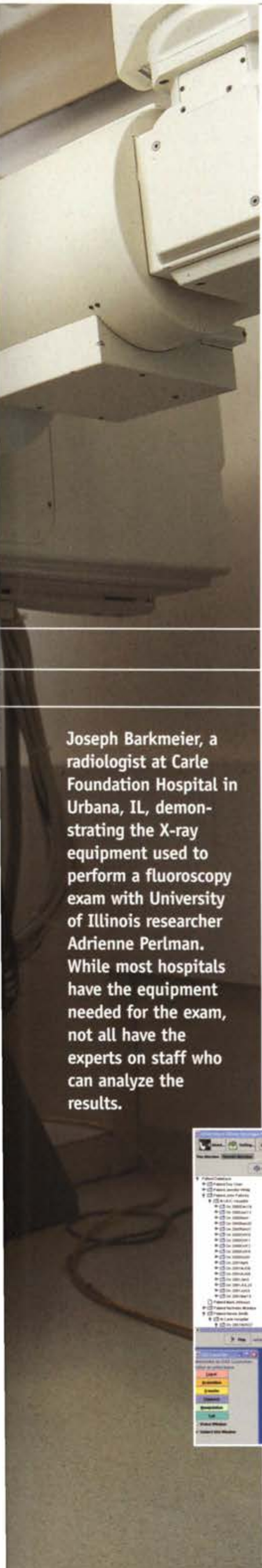
Paul Bode
Jeremiah Ostriker

by

Karen 'Green

Long-distance medicine

University of Illinois and NCSA researchers bring the medical specialists to the patients.



Joseph Barkmeier, a radiologist at Carle Foundation Hospital in Urbana, IL, demonstrating the X-ray equipment used to perform a fluoroscopy exam with University of Illinois researcher Adrienne Perlman. While most hospitals have the equipment needed for the exam, not all have the experts on staff who can analyze the results.

Early and accurate diagnoses and evaluations of medical conditions can save lives, money, time, and a whole lot of stress on patients and their families. Yet diagnosis and evaluation often depend on circumstances that have nothing to do with a patient's medical condition. Circumstances such as where a patient lives and what medical specialists are available in that area suggest that a person's zip code can be a good indicator of the quality of his or her medical care.

For example, dysphagia, or difficulty in swallowing, afflicts several hundred thousand people each year including the elderly, premature babies, stroke and cancer patients, and people with neurological disorders. Undiagnosed dysphagia can lead to respiratory problems, including life-threatening pneumonia caused by food or liquid in the lungs, and to malnutrition, which slows recovery from illness. Dysphagia can occur anywhere between the lips and the stomach. Oropharyngeal dysphagia, which results from mouth or throat problems, is generally diagnosed and treated by speech-language pathologists who have special expertise in this area.

Despite a large number of oropharyngeal dysphagia patients, many rural and small community hospitals have no experts on staff qualified to diagnose the condition. Some states with large rural areas have no more than a handful of dysphagia experts, mostly concentrated in larger cities. Unequal care levels depend on whether or not you are lucky enough to have the right medical professionals nearby.

Adrienne Perlman, a professor in the department of speech and hearing science at the University of Illinois at Urbana-Champaign, has studied, diagnosed, and treated dysphagia for 20 years. She recalls treating patients at a regional hospital in Iowa.

"The patients would often travel three, even four hours, to see me, sometimes by ambulance because they were so sick" says Perlman. "They would be exhausted by the time they'd see me. I remember thinking 'there's got to be a better way to do this.'"

Solving a diagnostic dilemma

Perlman eventually came upon a possible solution to her diagnostic dilemma: evaluating patients with dysphagia through remote, real-time medical assessments conducted over broadband Internet connections. As part of the NCSA/UIUC Faculty Fellows Program, Perlman has spent the past two years developing a method for capturing and transmitting high-quality video data from the fluoroscopic examinations that are used to assess a patient's swallowing. Such a system, she hopes, will make real-time remote assessment of fluoroscopy exams a common practice.

"We are testing the system with videofluoroscopic examinations of the oral and pharyngeal stages of the swallow in patients with dysphagia, but the system could be used for assessments in other areas of medicine," she says. "It is simply a system for interactive, real-time assessment of video images."

Weerasak Witthawaskul, a doctoral student in computer science at the U of I and Perlman's research assistant, and NCSA staff assisted Perlman by creating a Java-based interface that allows a desktop computer in a hospital X-ray suite to communicate with a similar computer in Perlman's laboratory on the U of I campus. This system allows Perlman to control the hospital-based PC from her lab and provides an interface for examining high-resolution MPEG versions of the videofluoroscopic images taken at the hospital.

Interface to Perlman's videofluoroscopic examination system.

A video image of a flouroscopy exam showing the tissue in the head and neck. The video player in the lower right of the image allows images that are transferred to the researcher's lab to be examined by running the video forward and backward and at varying speeds.

Patient with dysphagia in the process of swallowing. Some material is shown entering the patient's trachea (toward the front of the neck), while some enters the the esophagus (to the right of the trachea).

"The process is completely controlled from the computer in our lab" explains Perlman. "All the technician at the hospital has to do is turn on the computer in the X-ray suite."

Following the examination, Perlman is able to observe the swallow at full speed, in slow motion, or frame by frame on her laboratory computer. Moreover, she has the expertise to analyze the test data more precisely than most hospital clinics or labs. While staff at most clinics or labs can look at fluoroscopic images and determine whether cartilage, bone, or other structures move during the swallowing process, Perlman can measure displacement—how much and how long a structure moves and whether the movement is more or less pronounced than in previous exams. Displacement measurements can help determine both whether a dysphagia patient is recovering and the rate of recovery.

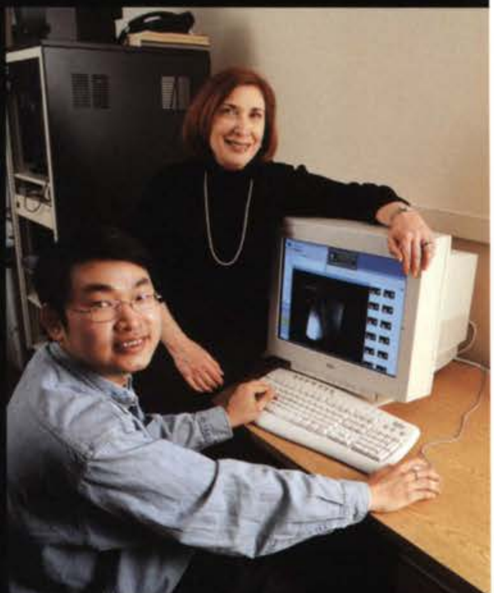
Testing the prototype

Videofluoroscopy with remote assessment is a relatively simple process that involves two major components. The first is a server PC equipped with video encoding hardware, located in the hospital X-ray suite. For the prototype system developed by Perlman and Witthawaskul, a 300-MHz Pentium computer was located in the X-ray suite at Carle Hospital in Urbana, IL. A 700-MHz Pentium computer, called the control and analysis computer, was located in Perlman's lab, about a mile from the hospital. The two machines were connected via the hospital's T1 Internet connection at a maximum speed of 1.5 megabits per second. Perlman, the dysphagia expert, directed the fluoroscopy exam from her lab, communicating with the hospital radiologist and the patient via a simple speakerphone connection. To operate Perlman's system, the hospital's radiologist merely turns on the server computer, then conducts a routine fluoroscopy exam. No special expertise is needed.

The examination takes place while the patient swallows a small amount of barium solution, which allows the fluoroscope to view the movement of the barium and of various structures in the mouth and throat. The fluoroscopic image is about as close as humans come to having X-ray vision. Skin and hair are transparent, while the skull and other bones, cartilage, and hollow tissues such as the esophagus and windpipe, are clearly visible. As the patient swallows, it is relatively easy to follow what happens. The hospital-based PC digitizes the videofluoroscopic images into an MPEG format and records the patient's swallowing activity in the highest resolution possible. Meanwhile, the video data are transmitted in real time to the control and analysis computer in Perlman's lab.

According to Perlman, the image quality during real-time transmission is adequate for directing the procedure, but does not offer the level of detail that she prefers for diagnosis. Real-time transmissions' low resolution results from the relatively limited bandwidth between the hospital and the lab.

During the examination, the control computer in Perlman's lab obtains and displays the video data in real time with only a three- to five-second delay—not enough to affect Perlman's ability to direct the procedure or cause undue radiation exposure to the patient. After the examination is completed, high-resolution fluoroscopic images, which were stored on the hospital computer during the examination, are transferred to Perlman's laboratory for complete analysis. Using these high-resolution images, Perlman is then able to look at the data frame by frame, search the video for specific frames, and adjust the brightness and contrast to better examine the data.



Adrienne Perlman and Weerasak Witthawaskul, University of Illinois at Urbana-Champaign.

Ending the tyranny of distance

Perlman's system could bring great change to medical establishments. Nursing home patients, who often arrive exhausted after traveling long distances for fluoroscopy exams, could avoid tiring travel and the expense of an ambulance. People fighting other illnesses or weakened from radiation treatments could receive expert medical assessments in their hometowns. Exams generally not offered at small and rural hospitals today—from assessments of swallowing functions to endoscopy, which evaluates structures such as the larynx, the esophagus, and the colon—could be easily available to patients who live hundreds or even thousands of miles from a major hospital. A person's zip code might no longer indicate the quality of medical care.

Perlman has high hopes for the system and is continuing her work with NCSA to upgrade the computer interface, improve the quality of the video from MPEG-1 to MPEG-2, and design a sophisticated security system that guarantees patient confidentiality. Eventually Perlman hopes to create a dysphagia portal and databank that would give researchers, educators, and clinicians worldwide access to dysphagia data. She sees the portal developing as a virtual workspace for swallowing experts where they will be able to collaborate with colleagues, discuss unique cases, examine data from around the world, and follow specific cases for months or years.

"What we've done so far is prove that this system can work," she says. "It is a service to the community and could be developed as a grid-based medical application."

This research is supported by the NCSA/UIUC Faculty Fellows program.

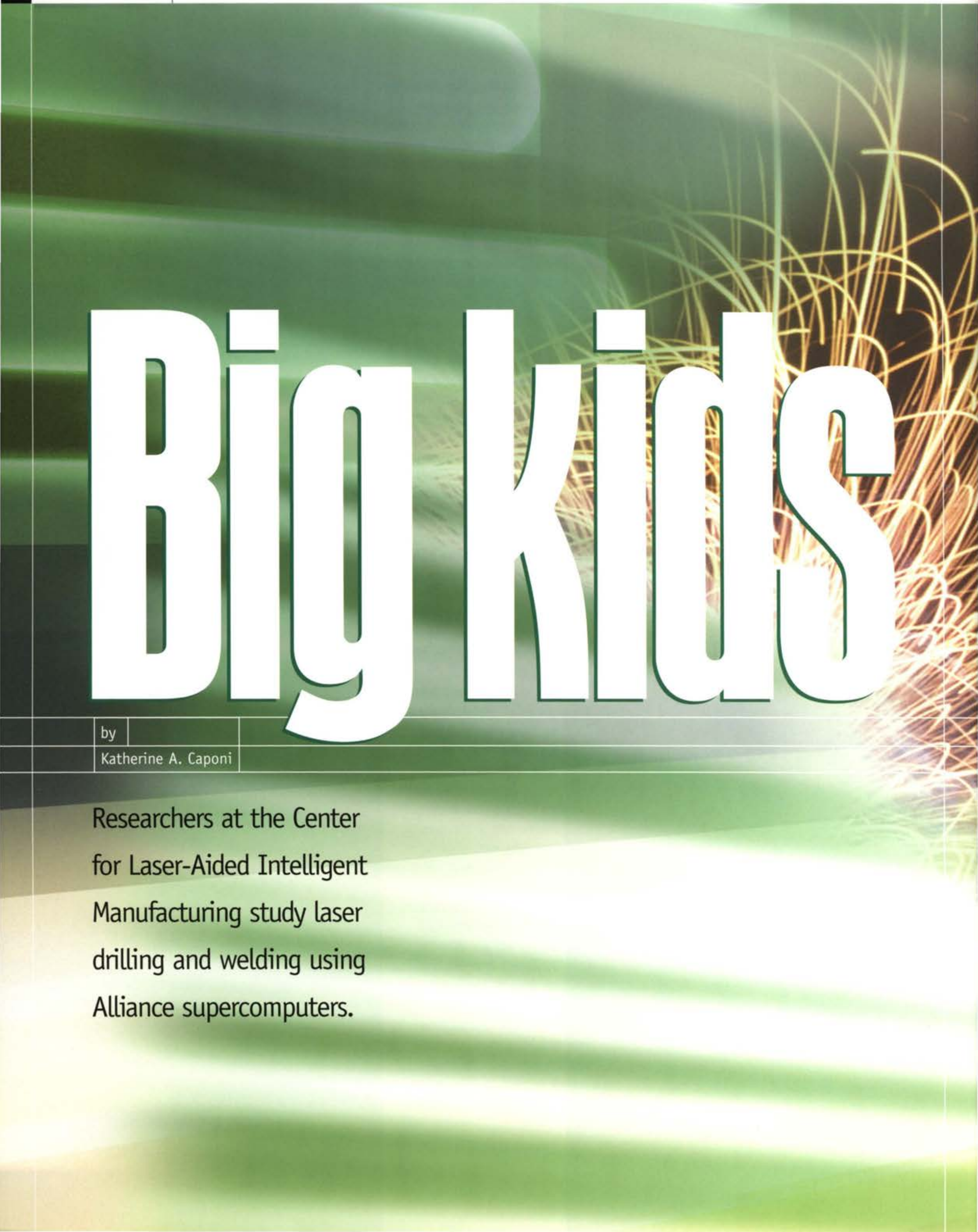
Access Online http://access.ncsa.uiuc.edu/CoverStories/dysphagia/

For further information:

http://white.shs.uiuc.edu

Team members

Adrienne Perlman
Weerasak Witthawaskul



Big kids

by
Katherine A. Caponi

Researchers at the Center for Laser-Aided Intelligent Manufacturing study laser drilling and welding using Alliance supercomputers.

"A child gets interested in light at an early age when she sees the first rainbow, or views a colorful spectrum created by diffraction through beveled glass, or burns paper by focusing sunlight through a magnifying glass. You always wonder about the mysterious ways light works. We are a bunch of big kids still playing with light to see how we can use pure light to society's benefit."

Jyotirmoy Mazumder displays a deceptively childlike delight in studying the pure, focused light of lasers. However, this "big kid" has a very grown-up mission. Laser drilling and welding are quickly replacing traditional methods of materials processing. The market for laser manufacturing constantly increases as new applications and technological advances give it increased potential for efficiency.

Jyotirmoy Mazumder, Pravansu S. Mohanty, and Hyungson Ki, Center for Laser-Aided Intelligent Manufacturing.

The problem is that laser processing is physically complex. During manufacturing, the material evolves through phases—liquid, solid, vapor, and plasma. Mazumder and his co-workers, Hyungson Ki and Pravansu S. Mohanty, of the Center for Laser-Aided Intelligent Manufacturing (CLAIM) at the University of Michigan, are studying the development of the phases to help streamline laser drilling and welding. They rely not only on their collective knowledge of physics, mechanical engineering, and materials science, but also on NCSA's Origin2000 supercomputer. The February 2002 issue of *The Journal of Laser Applications* features an article by the CLAIM team describing the results of their studies.

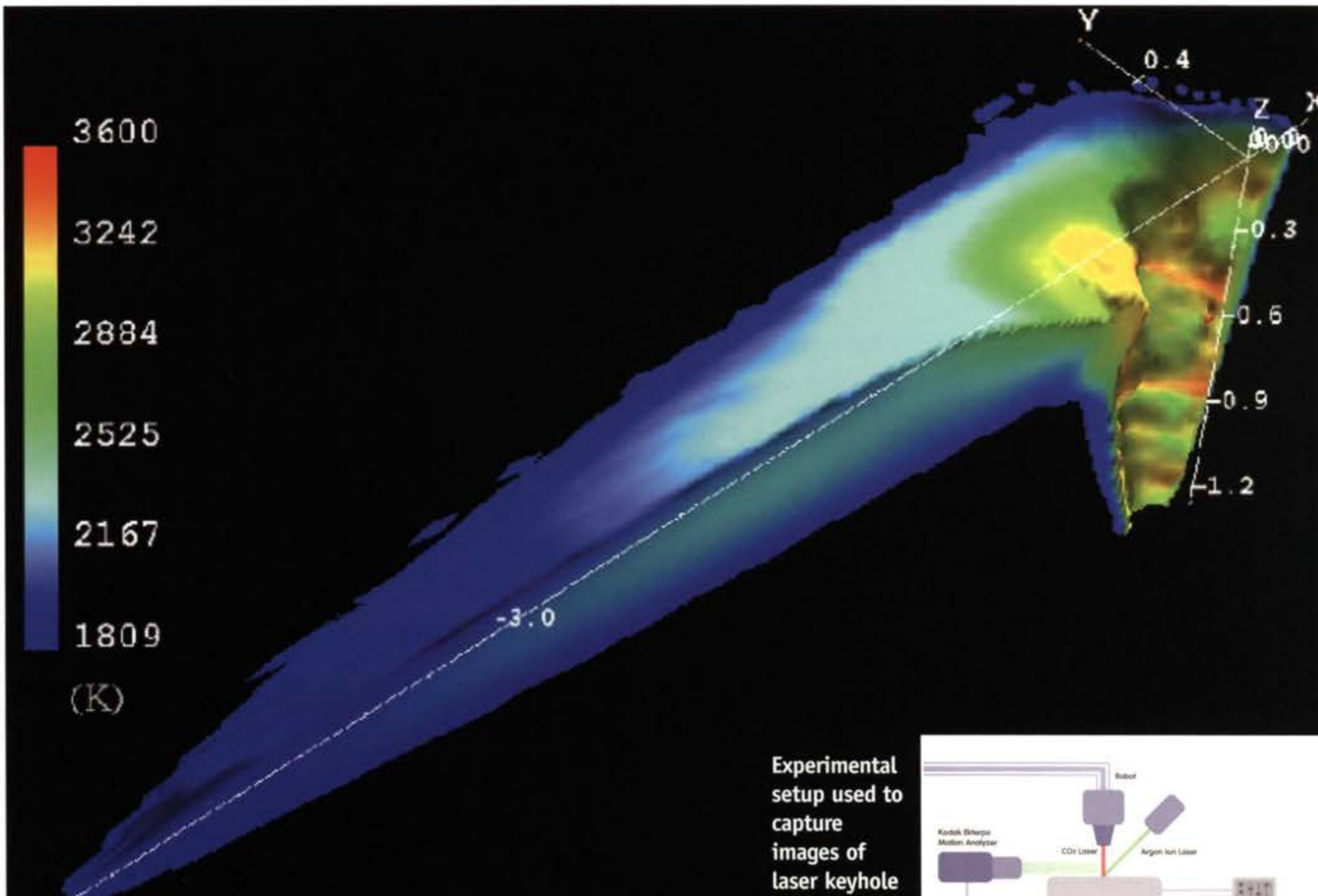
Trial and error made obsolete

Laser drilling, the removal of metal from a material to create a through-hole, is easily automated for speed and accuracy. This fact makes it an excellent tool for manufacturers looking for increased productivity and quality.

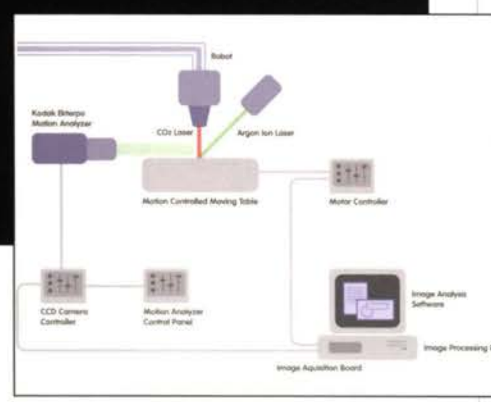
Laser welding is the joining of target materials through the conduction and radiation of absorbed laser energy. This process is faster than conventional welding and yields a more attractive finished appearance.

The current problem with both laser drilling and laser welding is that manufacturers often depend on trial and error to develop optimum processes. The main objective of the CLAIM scientists' work is applying atomic-level knowledge to materials processing and thereby reducing development time from concept to product.

Ki expresses enthusiasm and high hopes for the project, "I am so lucky studying one of the most exciting and challenging areas: laser materials interaction. Our goal is to understand the underlying physics thoroughly and, therefore, to fully realize the potential of lasers as the best manufacturing method."



Simulation of the weld pool shape after a full-penetration laser keyhole weld.



Experimental setup used to capture images of laser keyhole welding.

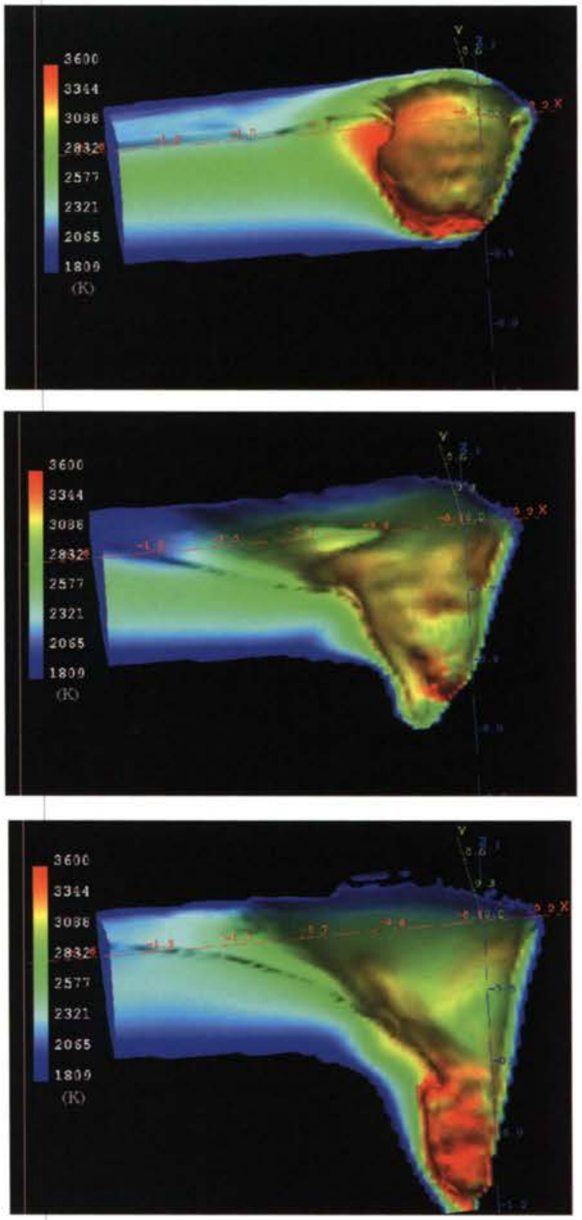
Unstable geometries

The CLAIM team employs a multidisciplinary approach in studying laser processing. Depending on the laser power, the target material in question can become extremely hot. The temperature can cause the form of the material to range between solid, melting, vaporizing, and boiling. These changes require an understanding of fluid flow and heat transfer. The scientists rely heavily on mechanical engineering to study these phenomena. However, other disciplines are critical to their research. They must understand temperature physics, the physics of plasma formation and laser-plasma interaction, and the microstructure of the weld through materials science.

After team members construct a theoretical understanding of the sciences involved, they develop computational models of two types of laser processing. The first is a simulation of laser drilling. The model includes fluid flow and heat transfer. Detailed knowledge of these phenomena is particularly vital to manufacturers because the processes can produce changes in the geometry of the through-hole and the finished product.

The second type of simulation is a computational model of laser keyhole welding. During the welding process, the high-energy density of the laser beam forms a keyhole, or vapor-filled cavity. The keyhole maximizes the energy spent by allowing a deep, narrow weld. However, the cavity is highly unstable, making it difficult to accurately simulate the keyhole's evolution. CLAIM's new laser welding model achieves accuracy by fully solving fluid flow, heat transfer, melting, and solidification. Their model accounts for changes in surface tension and fluid motion due to temperature variations and for factors in the pressure difference between the keyhole walls. The new knowledge of the ways these forces interact will allow manufacturers to optimize their laser processing capabilities.

This is not the first attempt to understand the nature of both laser drilling and laser keyhole welding. Most of the previous models assumed predefined hole shapes to make the problems simpler. The keyhole, however, is too dynamic to be calculated as a fixed object. The CLAIM team's study places no restrictions on the keyhole geometry. Instead, the cavity evolves as the consequence of other associated physics. The new model also demonstrates full laser penetration of the target material and multiple reflections within the keyhole. Every one of these processes plays a critical role in laser keyhole welding. Therefore, CLAIM's model is less susceptible to the unrealistic predictions of previous oversimplified models.



Simulated temperature variations during a full-penetration laser keyhole weld.

Photo of weld pool after full-penetration laser keyhole weld.

The simulations run on NCSA's Origin2000 platform. To date, the project has required 65,000 hours of supercomputing resources.

Through the keyhole

When the team finishes creating a welding model, they verify its accuracy against pictures taken of real laser welding in action. The scientists use a CO_2 laser beam as a heat source. During the laser welding process, an argon-ion laser beam illuminates the weld pool surface. They install a diffuser plate directly in front of the argon-ion laser so that the laser beam passes more evenly, greatly improving images of the molten surface.

Reflected images of the surface from the argon-ion laser beam pass through another filter located in front of a high-speed camera. A high-performance image-grabbing board in a computer acquires the images. Next, image analysis software processes it. The images appear on the computer screen and provide the team with information on the weld geometry and melt flow velocity. Due to the instability of the weld area, the experiment is repeated ten times and results are averaged. The images prove that the models designed by the team reasonably match the actual process of laser welding.

The process allows the CLAIM team to help shape lasers' impact on manufacturing. The newly gained scientific knowledge and the team's models of laser drilling and welding will help the industry better predict the effects of various process parameters. Their contributions will also eliminate mistakes, thereby reducing scrap and producing higher quality end products.

Mazumder's own words best capture the big picture of laser potential: "Civilization is often identified with a form of energy. Wind power started navigation. Steam power started the Industrial Revolution. What is around the corner for the laser light?"

This research is supported by the Office of Naval Research and General Motors.

Access Online http://access.ncsa.uiuc.edu/CoverStories/laserkeyhole/

For further information:

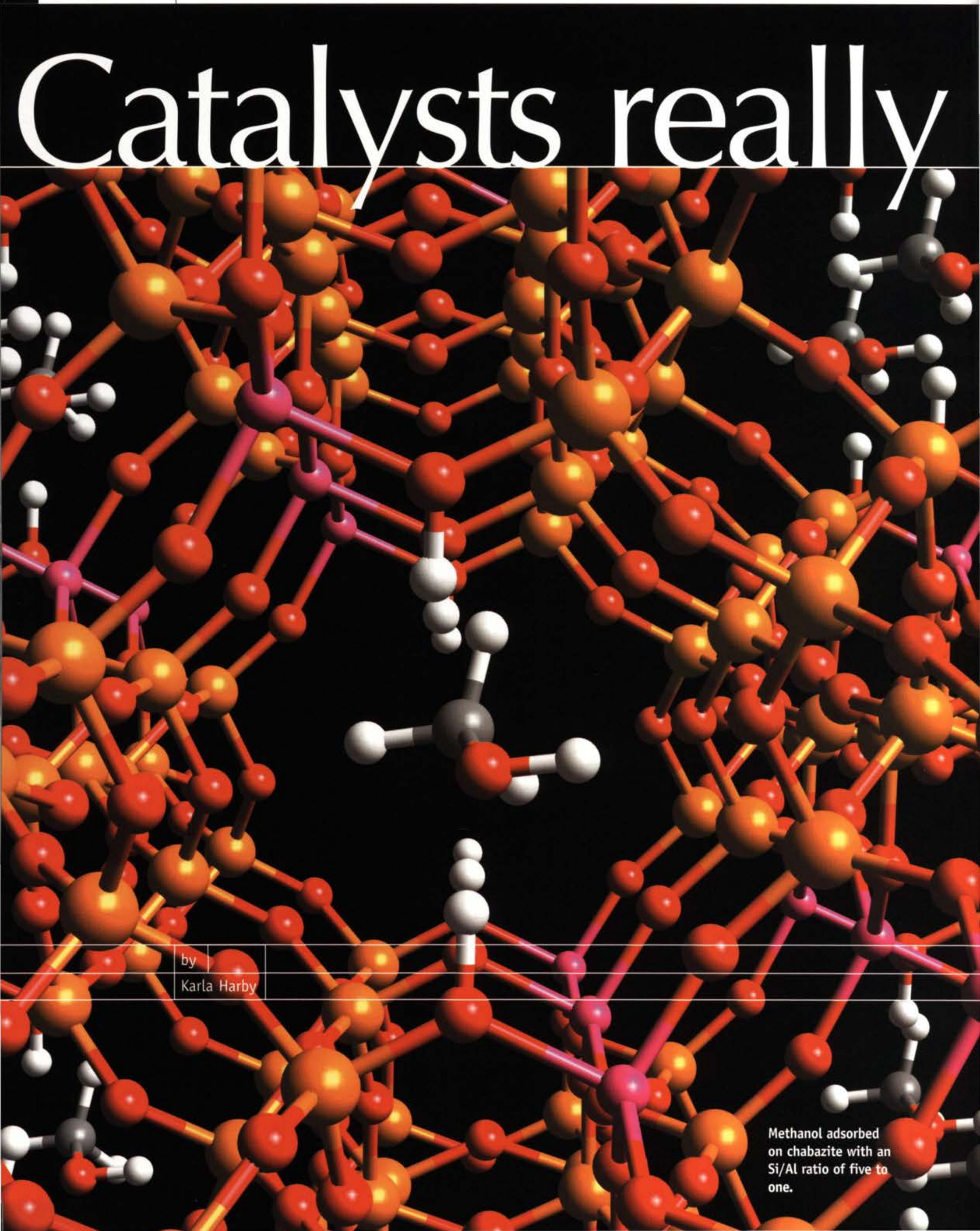
http://claim.engin.umich.edu/

Team Members

Hyungson Ki
Jyotirmoy Mazumder
Pravansu S. Mohanty

Catalysts really

by
Karla Harby



Methanol adsorbed on chabazite with an Si/Al ratio of five to one.

rock

Computational methods are helping computational chemists unravel the complexities of inorganic catalysts with possible implications for ozone depletion and the automotive industry.

Chabazite.

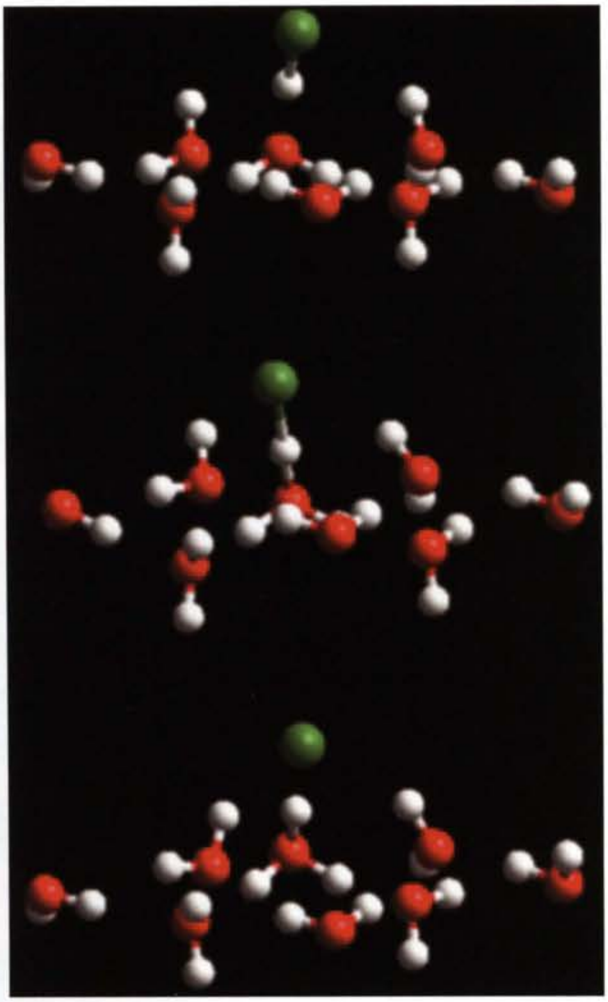
Chabazite is a rare mineral with a beauty that makes it a rock collectors' favorite. Creamy colored or pinkish with a vitreous sheen, it is pressed into nearly cubic crystals when volcanic rocks are subjected to the heat and pressures of metamorphosis.

Although chabazite looks impressively solid sitting on a coffee table, on the atomic level it has properties possessed by all zeolites—it's full of holes. Zeolites, a class of natural and synthetic minerals possessing large, vacant spaces in their crystalline structure, provide tunnels and hideouts for such atoms as potassium, sodium, and calcium and even for molecules like water and ammonia. This property makes zeolites useful for things such as water purification and softening, removing radioactivity from spent nuclear fuel, and controlling kitty litter odor.

The cavities in a zeolite's structure also help explain its effectiveness as a catalyst. A catalyst is a substance, in this case an acidic solid, that facilitates chemical reactions without itself being changed. Not much is currently known about these zeolite caves on the atomic level, including how they interact with the atoms that enter their passages. Successful spelunking here could have ramifications far beyond the contentment of the household cat.

"Zeolites are rather large, complex systems. They're analogous to enzymes," says David White, a chemistry professor at the University of Pennsylvania. "The big question is: What kind of chemistry goes on in small cavities?" Because cells also contain complex networks of cavities, a better understanding of the chemistry of zeolites could reveal much about the chemistry of biological systems.

Bernhardt Trout, professor of chemical engineering at the Massachusetts Institute of Technology, White, and other collaborators are using the Alliance's SGI Origin2000 supercomputer at NCSA to simulate catalysis computationally. They chose chabazite as their archetype zeolite because it's used in industry to convert methanol to olefins. Despite having rather complex zeolitic systems, chabazite is small enough (only 36 atoms) to be successfully modeled by supercomputers, yet big enough to yield important information.



Snapshots from a Car-Parrinello molecular dynamics simulation at 150 K depicting HCl adsorbed on a model ice surface at 0, 0.17, and 0.43 picoseconds. The top configuration (at 0 ps) corresponds to the optimized geometry of molecular HCl on ice. Only the top bilayer of the ice model is shown in each frame.

Trout is also using the Origin2000 to study both catalytic behavior relevant to the catalysts used in cars' catalytic converters and the chemistry of ice crystals. Understanding how ice in the stratosphere reacts with other compounds could offer insights into ozone depletion and how to prevent it.

Simulations surprise

Trout came to Alliance resources with specific questions in mind. In less than a year he had already obtained a key—albeit preliminary—finding. Chabazite has four different oxygen sites and, consequently, four different acid sites available for absorbing other molecules. Scientists previously thought these various acid sites had substantially different energetics—in other words, that the energy required for chemical reactions varied. This assumption suggested that the four sites could differ greatly in their chemical activity.

But simulations on the Origin2000 have so far revealed quite the opposite. Among the four sites, the energetics for catalytic activity is the same, Trout says.

"[Zeolite chemistry] can be very fascinating," says White, whose research group designed experiments to check the validity of Trout's computer simulations with chabazite. "If the supercomputer is important to us, it's because it can be predictive."

He adds: "Much of the calculation in chemistry is not really predictive, so experiments are done to get a model. But physicists can do that—they predict when the earth is going to end, and we sit here, waiting. Chemists have not been able to do this, because chemical systems are, in a way, much more complex."

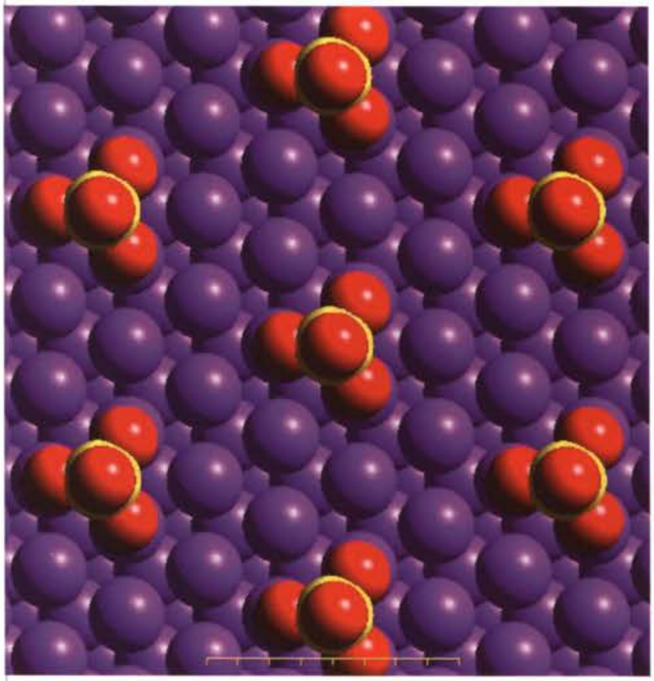
Reducing auto emissions

Although Trout's work has focused on the chemistry of zeolites, he's quatitatively studying other important catalysts as well. In a joint project with the Ford Motor Company, Trout has been using computational catalysis to see whether sulfur resistant catalysts in cars' catalytic converters can be developed for lean-running engines.

A lean engine runs with a high air-to-fuel ratio, or an excess of oxygen (O_2). "Lean in general is a good thing because you get more efficiency," Trout says. "If you can get more efficiency, you decrease emissions in addition to saving money on fuel."

A new and potentially promising catalyst for lean-running engines is composed of platinum and barium oxide (BaO). Unfortunately, a BaO catalyst cannot be used today because, under lean conditions, the sulfur present in gasoline oxidizes on the catalyst's platinum to produce sulfur trioxide (SO_3). This byproduct then poisons the BaO, rendering the whole catalytic material useless for absorbing the nitrogen oxide (NO_X) emissions in air pollution.

But, there might be a way to design catalysts that resist damage from sulfur. "We're on our way to computing about 100 configurations" for automobile catalysts, Trout says. "We have the energetics, and we're working on kinetics of the SO_2 oxidation reaction."



Molecular chemisorbed SO_4 on a platinum (111) surface.

The Trout research group in front of MIT's Killian Court.

Probing the ozone hole

In collaboration with Mario J. Molina, an institute professor also at MIT, Trout is using Alliance computational power to explore how chemical reactions occur on the ice crystals of stratospheric clouds.

That the subject is under study at all is noteworthy. Until the 1980s, chemists thought that ice was chemically inert—that when dilute solutions froze, pure ice crystals grew and the impurities remained largely in the liquid phase. But work by Molina and others suggested that ice has a layer of disorder on its surface that engages in chemical reactions.

"I stay away from the word 'melting,'" Trout comments about this layer because melting implies the conversion from a solid to a liquid. "This is just the interfacial region. In an ice cube in water, you see the ice, you see the water. There's a region between the two that looks rigid to the eye, but it isn't so rigid."

While everyone now agrees that ice—including the ice crystals in clouds—participates in chemical reactions that contribute to ozone depletion, the mechanisms involved remain controversial. Trout speculates that one particularly active site on ice may explain activity without resorting to the disordered-region hypothesis. In other words, focusing on disorder on the surface of ice may not be needed; a perfectly ordered region may explain this chemistry. If confirmed, that would be a fascinating new finding.

"From what we've been working on, we don't have something to solve the ozone [depletion] problem, but then no one else does either, so we try not to feel too bad about that," Trout allows. But, he adds, someday computational catalysis may help us "know better the consequences of what humans produce and make informed on decisions about what we are sending up there [into the ozone layer]."

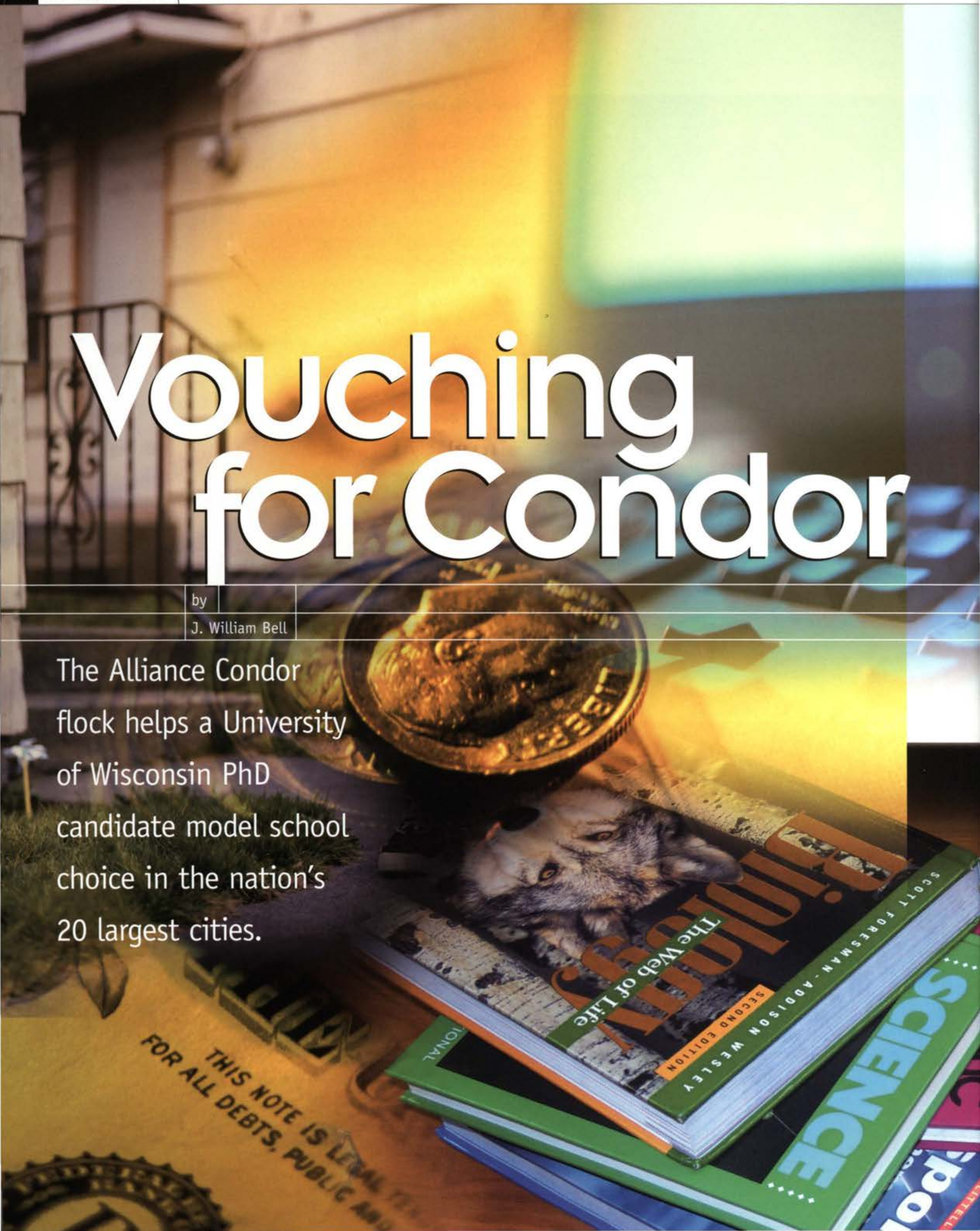
In the meantime, computational catalysis has already proven its power as a new instrument for helping scientists understand a wide variety of important chemical behaviors at the molecular level. "We [theorists] don't work on a thing that can't be validated," Trout explains. But "the level of detail we can get with computers is not possible in the laboratory."

This research is supported by the National Science Foundation, Ford Motor Company, and NASA.

Access Online http://access.ncsa.uiuc.edu/CoverStories/zeolites/

For further information:
http://troutgroup.mit.edu

Team members
Mario J. Molina
Bernhardt Trout
David White



Vouching for Condor

by

J. William Bell

The Alliance Condor flock helps a University of Wisconsin PhD candidate model school choice in the nation's 20 largest cities.

A contentious but common part of many education reform plans, vouchers help parents pay private school tuition using municipal, state, or federal funds. Advocates say vouchers give parents the opportunity to educate their children as they see fit and force public schools to improve by introducing competition for funding. Opponents contend that voucher plans jeopardize a fundamental public good of offering everyone high-quality public schooling; the dollars given to vouchers are dollars lost for strapped public schools.

To complete her dissertation at the University of Wisconsin, Maria Ferreyra, a PhD candidate in economics, explored the behavior of city dwellers as they chose their houses, neighborhoods, and public, private, or Catholic schools. With the Alliance Condor flock at the University of Wisconsin and an economic model developed by Duke University's Tom Nechyba, she analyzed the ways in which introducing school voucher programs in the nation's 20 largest cities might influence where people live, how they spend their money, and what schools they send their children to.

"Currently, many households opt out of the public school system to send their children to private schools," Ferreyra says. "These households pay tuition in addition to the property taxes used to support local public schools. There are also many households that would prefer private schools but face financial constraints that restrict them to public schools."

Voucher programs are scarce, which makes judging their effects and plotting their future difficult. Only Milwaukee, Cleveland, and the state of Florida have test programs, according to a December 2001 report by *Education Week*, and all are nascent, small-scale efforts. Ferreyra's work is neither a red light nor a green light. It is, however, an excellent tool for answering questions about potential large-scale voucher programs that haven't been implemented to date.

How does it work?

To answer these questions, Ferreyra used what is known as a general equilibrium model to isolate the system's main agents. In Ferreyra's case, agents included families, schools, school districts, and the state government. Mathematical equations represent what these agents are seeking, under what circumstances they will pursue those goals, and how one agent's pursuit influences another's situation.

The thorny equation that determines a family's behavior, for example, includes varying interest in school quality, housing quality, schools' religious orientations, and consumption of all other goods. This equation is known as their utility function. Another equation represents families' budgetary constraints. Families' actions are ruled by their attempts to get the most of each aspect of the utility function within their budget. If they have a high desire for a good public school, they'll forgo a better house in a lesser school district. If they want a Catholic school, they'll put money into that instead of a mansion. If vouchers are available, a family may not have to worry about the school district they're in when house shopping.

Another equation determines school quality, which is a function of peer quality and dollars spent per student. These factors are, in turn, determined by other, ever-changing factors. In this simplified model, peer quality equals the average income of families whose kids attend the school, and public schools' spending is funded with property taxes, which the districts' families vote on.

Until each family finds its perfect situation and the housing markets settle—until the model reaches equilibrium—the families are on the move. And the computer model chugs away, tracking the fantastic interplay among the various equations.

"Imagine you dropped the cities' citizens from an airplane," Ferreyra says. "The wealthy who don't have an interest in religious education all move to the district with the best housing, and, because public-school spending depends partly on property taxes, they end up with public schools that spend the most per student. In the meantime, other people are trying to find the best place for themselves. Most people will not be happy where they land. And everyone is voting on taxes and changing the nature of all the districts and their public schools."

It's not just a matter of people finding their place; they're changing the nature of the place as they go. "The only thing that stays constant is housing quality. Everything else is moving parts," Ferreyra explains. "This is precisely why we want a general equilibrium model. It allows us to look at different markets—the housing and schools markets, in this case—and how they change as people move, choose schools, and vote on property taxes. With the model, we get to see how the markets change when a large fraction of families are involved—unlike current real-world programs, which happen at a much smaller scale."

What is it based on?

The model provides a plausible depiction of reality through the previously described equations, representing families, schools, districts, and states. Some data for these equations are provided. The data establish things like the income distribution among families in each of the 20 cities Ferreyra looked at, the number of Catholic families, housing quality in the different neighborhoods and districts, and how much money per student the state gives to public schools. For this information, Ferreyra relied on several sources including the 1990 census, a general social survey that tracks religious preferences, and a guide to school district spending.

Other parameters of the equations are missing. Some of them correspond to more ethereal traits that drive families—how much a family values a religious education or how much they value house quality. Ferreyra's task was first to quantify these traits.

To determine the values, Ferreyra tried thousands of sets of plausible hypothetical parameter values, running the model of each city to equilibrium for each set of values. The data that came out after the model reached equilibrium included new figures for property values, school spending, and income—as well as some data that were not provided, such as the number of students in private nonreligious schools and the number of students in Catholic schools.

Ferreyra compared these data to real-world statistical data to determine the quality of the hypothetical values she had inserted to represent the parameters. Choosing values that yielded equilibrium conditions that best matched the real-world data, this process gave her a glimpse of families' thinking and the situations that produced varying levels of school quality.

Maria Ferreyra, University of Wisconsin.

Then, using those optimal values, she added features to the model to examine the same economic system, now with vouchers. Having already quantified the unknown parameters, she could be confident that the resulting picture of families using vouchers would be accurate.

Ferreyra's model is the progeny of a model built in the mid-1990s by Tom Nechyba. Nechyba began the model as part of his dissertation at the University of Rochester, introducing schools to the mix later. Ferreyra added the functions that track families' religious interest, represent the distinction between Catholic and nonreligious private schools, and incorporate vouchers.

These additions are significant because of the prominence of religious schools. According to Ferreyra, about 85 percent of enrollment in private schools in grades 9 through 12 is in religious schools. About 60 percent of that enrollment is in Catholic schools alone.

"Maria fleshes out that it's not all about peer quality or dollars or a school quality hierarchy. Yes you care about peers, yes money, but many also care about religion. And they care about all these things to varying degrees," says Nechyba, now an associate professor of economics and public policy studies at Duke University.

Ferreyra also estimated the model instead of simply calibrating it. Calibrating would have involved looking at a single city. It would have still allowed her to derive optimal values for the model's parameters and to compare the values' implications to real-world statistics, but it would have also lacked scope. By estimating the model and looking at 20 cities, she proved the reliability of the model in a more general way.

"In estimating," Ferreyra says, "you use more data, search more exhaustively for the optimal parameter values, and provide a measure of how good the final parameter values are. You get a much broader sense of quality. And since those values are used to simulate voucher experiments, we want to ensure their quality as much as we can."

Why does it require Condor?

A run of the model is not as taxing as many classical supercomputing tasks. Running a set of parameter values to equilibrium for all 20 cities requires only about 20 minutes on one of the machines in the University of Wisconsin's Condor flock, which pools the power of desktop workstations and Linux clusters across Wisconsin's campus.

But Ferreyra, with the help of Condor team members including Peter Keller and Zach Miller, ran the model about 50,000 times to find the optimal parameter values, using as many as 200 processors at the same time. This computation took about a week, and, by the time Ferreyra was finished testing the model and working the bugs out, she had run the model about 15 times. Working on a single-processor desktop computer, the computations would have taken about 24 years, according to Keller.

"This is a classical Condor application—a very large number of independent computations that explore a parameter space. Condor provides the resources and management capabilities needed to support studies like this," says Miron Livny, a computer science professor at Wisconsin, head of the Condor project, and leader of the Alliance's Partnerships for Advanced Computational Services.

After estimating the 20-city model, Ferreyra simulated the impact of vouchers in metro Chicago. She found that families using vouchers migrated to neighborhoods with lower housing quality, that vouchers usable at both Catholic and nonreligious private schools increased enrollment in both types of schools, that vouchers restricted to nonreligious private schools caused a smaller increase in private school enrollment, and that, in systems where use was restricted to nonreligious schools, enrollment in Catholic schools declined as the dollar amount of vouchers increased. She also found that low voucher levels of around $2,000 per year helped mostly the middle class, but higher voucher levels aided both the poorer and the richer as well. Finally, she discovered that public schools can be positively or negatively affected, depending upon the school district they are in.

These early insights are not the only upside to this extensive modeling project, though.

"A problem like this is very hard to analyze without a general equilibrium model like this one," says Nechyba, "and without computing resources [like Condor]. As we have successes like Maria's, a larger number of problems are recognized as benefiting from a general equilibrium approach, and we can expand the approach to new ideas. Projects like this help persuade others that this is one very useful way of thinking about the world."

This research is supported by the University of Wisconsin Department of Economics and the Robock Award in Empirical Economics.

Access Online http://access.ncsa.uiuc.edu/CoverStories/vouchers/

For further information:

http://www.econ.wisc.edu/~mferrey/

What is the GRID?

Dan Reed
Director, *National Computational Science Alliance*

Director, *National Center for Supercomputing Applications*

Francine Berman
Director, *National Partnership for Advanced Computational Infrastruture*

Director, *San Diego Supercomputer Center*

Paul Messina
Chair, *Global Grid Forum Advisory Committee*

Former Director, *California Institute of Technology's Center for Advanced Computing Research*

Rick Stevens
Chief Computational Architect, *National Computational Science Alliance*

Director, *Argonne National Laboratory's Mathematics and Computer Science Division*

Ian Foster
Associate Director, *Argonne National Laboratory's Mathematics and Computer Science Division*

Professor, *University of Chicago*

Ed Seidel
Head, *Max Planck Institute for Gravitational Physics' Numerical Relativity Group*

Senior Research Scientist, *National Center for Supercomputing Applications*

Bill Johnston
Project Manager, *NASA's Information Power Grid*

Senior Scientist, *Lawrence Berkeley National Laboratory*

Charlie Catlett
Chair, *Global Grid Forum*

Executive Director, *TeraGrid project*

Miron Livny
Professor, *University of Wisconsin*

Head, *Condor high-throughput computing project*

Bill Feiereisen
Director, *Los Alamos National Laboratory's Computer and Computational Sciences Division*

Former Director, *NASA's Numerical Aerospace Simulation Systems Division*

Grids are both a dream and a tool for realizing even larger dreams. Today, most grids are small and research oriented. They're early forays away from the coast and into a vast, unexplored ocean. Tomorrow, the grid will be a single, sustained engine for scientific invention. It will link petaflops of computing power, petabytes of data, simulation and modeling codes of every stripe, sensors and instruments around the globe, and tools for discovering and managing these resources. At your desktop and at your whim, you'll have access to the world and its computing assets. What you do with them is the larger dream.

This multimedia presentation introduces some of the leaders in grid development. They describe what the grid will become, how it will get there, and what it will allow scientists to do.

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NCSA
National Computational Science Alliance
University of Illinois at Urbana-Champaign
605 East Springfield Avenue
Champaign, IL 61820-5518

http://alliance.ncsa.uiuc.edu